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DIFFICULTY AND POSSIBILITY OF

KINETIC THEORY OF QUANTUM-MECHANICAL SYSTEMS

Part II — The Quantum-mechanical

Liouville Equation and Its Solutions

by

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and
APPLIED MECHANICS

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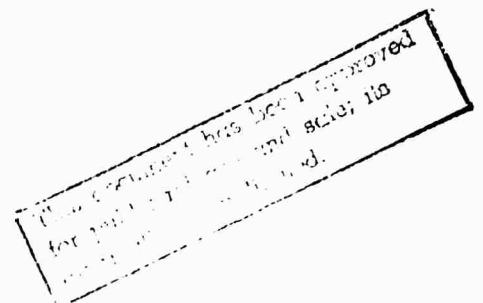Part II - The Quantum-mechanical

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KINETIC THEORY OF QUANTUM-MECHANICAL SYSTEMS

Part II - The Quantum-mechanical
Liouville Equation and its Solutions[*]

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Toyoki Koga[**]

SUMMARY

The theme of this report is a problem of correlation, as
is illustrated in section I by considering the two-electron
problem according to the Schrodinger equation. In section II,
the Schrodinger equation is reduced to a partial differential
equation which is equivalent to the classical Liouville
equation, to the approximation of nullifying h^2 in the former.
An energy eigen-function of the Schrodinger equation correspnds
to the representation of a micrccanonical ensemble of classical-
mechanical systems in the phase space. For example, the energy
eigen function of the electron in a one-electron atom corresponds
to a microcanonical ensemble of single-particle systems in the
classical-mechanical sense. The uncertainty existing in the
quantum-mechanical representation of a particle is two-fold:
A part of the uncertainty stems from our intention to describe
the behavior of the particle, which is likely to have an
extension in the six-dimensional phase-space, in

terms of the concept of classical material point; it also
stems from the situation that we are treating an ensemble
when we assume that we are treating a single particle.
If this were not the case, we would have no way to explain
strange kinetic-theoretical phenomena, which really exist
and fail to arise from the application of conventional
theories. In view of the above, the kinetic theory of quantum-
mechanical systems is difficult to rely on standard solutions
of the Schrodinger equation. Rather, at the present time, it
seems most reasonable to utilize quasi-classical models of
particles. The present discussion provides some legitimacy
and significance to those models. Finally, the present
interpretation of quantum mechanical phenomena provokes no
disturbance in the conventional structure of the quantum-
mechanical interpretation of the Schrodinger equation, so
far as the conventional application of solutions of the
equation is concerned.

I. INTRODUCTION

In Part I of this report, it is discussed that there is
a possibility of kinetic theory of quantum-mechanical systems,
since there are evidences that the validity of the Pauli
principle is localized. Nevertheless, we soon realize that
it is not so easy to consider kinetic theory of quantum-
mechanical systems. The situation is explained in the follow-
ing.

Suppose that we have a two-electron system, as the simpl-
est case. We may write down the Schrodinger equation for the
system. This two-body problem is quite different from the

classical two-body problem. In the present case, we cannot define the relative velocity, the center of mass, etc. of the two electrons, and hence there is no way to simplify the problem by changing the coordinate system. (If one of the two particles were a heavy atom, there would be a way of justification of doing so, as we really do for calculating the electron energy of an atom.) The Hartree-Fock method has nothing to do about the difficulty, since we do not want to introduce the additional statistical sense all at once. Finally, we suppose that, to the zeroth approximation, the wave function of each electron is a plane wave: $\psi_o^1(r_1)$, $\psi_o^2(r_2)$. Then we construct a wave function for the whole system,

$$\psi_o = \psi_o^1(r_1)\psi_o^2(r_2) - \psi_o^1(r_2)\psi_o^2(r_1)$$

To the next approximation, we write $\psi_1 = \psi_o + \varphi$, and substitute ψ_o for ψ in the interaction term of the Schrodinger equation, and simply φ in the other terms. It is not yet a simple equation, but we suppose that we get a solution for φ . Is this the correct solution for the present problem? It is easily seen that this solution implies that the two electrons are interacting mutually at any time and anywhere in the same way; each electron appears to have been ground to a sort of powder of extremely small grain and spread uniformly in the entire space. Is this the real mode of the interaction between two electrons? The situation does not change as depending on the amount of energy contained in the system. In other words, we cannot switch this to the classical two-body problem, as long as we use those wave functions.

We remember that we meet a similar situation in the classical kinetic theory, if we use an ensemble representation of a system. (Ref.1). But we cannot simply conclude that the

situation of quantum-mechanical kinetic theory is analogous to
the classical case. In this report, we investigate the
matter more closely, by utilising the quantum-mechanical Liouville
equation which is derived from the Schrodinger equation, and
attempt to find a feasible way of kinetic theory of quantum-
mechanical systems.

II. DEDUCTION OF THE LIOUVILLE
EQUATION FROM THE SCHRODINGER
EQUATION

It has been known that the Wigner equation which is derived
from   the   Schrodinger equation by a method of Fourier
transformation is equivalent to the classical Liouville equa-
tion to the approximation that the term involving h is ignored
and the potential is expandable in a Taylor series, and its
first derivative is retained. Ref.2. However, the procedure
of the derivation is not analogous to the classical one, and
hence it is difficult to see the physical c orrespondence
between the two. In this section we also derive a partial
differential equation from the Schrodinger equation. This
equation is equivalent to the classical Liouville equation to
the approximation of nullifying h^2, not h, in the former.
Besides, the procedure of derivation of this quantum-mechanical
Liouville equation is much analogous to the derivation of the
classical Liouville equation according to the Hamilton
formalism. Hence we can see rather easily the correspondence,
physical and mathematical, between the two equations, classical
and quantal. In the following, the introductory part, down

to Eq.(2.3)', is well known. See Ref. 3.

   We write the Schrodinger equation for a particle in
a   potential field U as follows:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + U\psi \tag{2.1}$$

$$\hbar = h/2\pi$$

We substitute in the above

$$\psi = a \exp(iS/\hbar) \tag{2.2}$$

where a and S are real functions of t and $\vec{r}$; $\vec{r} = x,y,z$.
(Any function which can be expressed as a sum of real and
imaginary parts may be written as (2.2).) On considering
the real part and the imaginary part in the equation separately,
we have

$$\partial S/\partial t + (\text{grad } S)^2/2m + U - \hbar^2 \Delta a/(2ma) = 0 \tag{2.3}$$

$$\partial a^2/\partial t + \text{div}(a^2 \text{grad } S/m) = 0 \tag{2.4}$$

To the approximation of ignoring $\hbar^2$, Eq.(2.3) yields

$$\partial S/\partial t + (\text{grad } S)^2/2m + U = 0 \tag{2.3'}$$

   In the following, it will be shown that first Eqs.(2.3)' and
(2.4) lead to the classical Liouville equation and second Eqs.(2.3)
and (2.4) lead to a partial differential equation which may be
called the quantum-mechanical Liouville equation.

   1. The classical Liouville equation.

   Equation (2.3)' is the Hamilton-Jacobi equation. The H-J
equation implies Newton dynamics under certain additional
conditions. Without the conditions, the H-J equation is a
differential equation of broader implication. We first derive
the Liouville equation in the classical sense, by introducing
the additional conditions.

We suppose that we obtain a "complete" integral of Eq.(2.3)',
a solution containing three arbitrary constants in addition to
an additive constant:

$$S(\vec{r}, t, \alpha_1, \alpha_2, \alpha_3) + S_0$$

See Ref.[4]. From now on, we shall ignore constant S_0. Then
we define $\vec{p}$ and β_1, β_2, β_3 by

$$\vec{p} = \text{grad } S \tag{2.5}$$

$$\beta_1 = -\frac{\partial S}{\partial \alpha_1}, \quad \beta_2 = -\frac{\partial S}{\partial \alpha_2}, \quad \beta_3 = -\frac{\partial S}{\partial \alpha_3} \tag{2.6}$$

In order to let $\vec{p}$ imply momentum, it is necessary to put that

$$\frac{d\alpha_\nu}{d t} = 0, \qquad \frac{d\beta_\nu}{dt} = 0, \qquad \nu = 1, 2, 3 \tag{2.7}$$

(These conditions are not contained in the H-J equation.)
According to (2.5), the components of $\vec{p}$ are functions of $\vec{r}$, t
and the α's:

$$p_x = p_x(\vec{r}, t, \alpha)$$

$$p_y = p_y(\vec{r}, t, \alpha) \tag{2.8}$$

$$p_z = p_z(\vec{r}, t, \alpha)$$

Similarly, the β's are

$$\beta_1 = \beta_1(\vec{r}, t, \alpha)$$
$$\beta_2 = \beta_2(\vec{r}, t, \alpha) \tag{2.9}$$
$$\beta_3 = \beta_3(\vec{r}, t, \alpha)$$

By eliminating x,y,z from those six equations, we may obtain
the p's as functions of the α's and β's and t:

$$p_x = p_x(\alpha, \beta, t)$$
$$p_y = p_y(\alpha, \beta, t) \qquad (2.10)$$
$$p_z = p_z(\alpha, \beta, t)$$

and subsequently, Eqs.(2.8) yield

$$x = x(\alpha, \beta, t)$$
$$y = y(\alpha, \beta, t) \qquad (2.11)$$
$$z = z(\alpha, \beta, t)$$

These six functions give the trajectory of a particle in accordance with the Newton dynamics. Since there are six constants, the α's and β's, involved in those functions of t, one may choose the p's at time t as independent of the choice of x,y,z. If we define H by

$$H = (\text{grad } S)^2/(2m) + U = p^2/2m + U$$

then, according to (2.3)' and (2.5), we have

$$(d\vec{p}/dt)_r = - \text{grad } H = -\text{grad } U \qquad (2.12)$$

where ( )$_r$ means that the derivative is made under the condition that r is fixed.* (If we wish to do so, we may take the α's for the three initial coordinates and the β's for the three initial components of momentum.)

We consider Eq.(2.4) in terms of the solution of Eq.(2.3)' considered in the above. Considering (2.5) and that $\vec{p}$ and $\vec{r}$ are mutually independent, in accordance with (2.10) and (2.11), we write for Eq.(2.4)

$$(\partial a^2/\partial t)_r + (\vec{p}/m) \cdot \text{grad } a^2 = 0 \qquad (2.4)'$$

In this presentation, $\vec{p}$ is a function of the α's, β's and t. By solving this equation, we suppose, we obtain a "complete"

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*This is the initial definition of $\partial/\partial t$ in Eq.(2.3).

solution which contains three more additional constants

δ_1 , δ_2 , δ_3 :

$$a^2 = \rho_o (\vec{r}, t, \alpha, \beta, \delta) \tag{2.13}$$

where α means the α 's. By means of (2.10), however, we may
eliminate either the α 's or the β 's and bring in the p's
instead. Suppose we eliminate the α 's. Then we obtain a
function of $\vec{r}$, $\vec{p}$, t, β, δ for a^2:

$$a^2 = \rho(\vec{r}, \vec{p}, t, \beta, \delta) \tag{2.14}$$

If we rewrite Eq.(2.4)' in terms of this function, we have to
write

$$\partial /\partial t + (dp/dt)_r \cdot \partial /\partial \vec{p}$$

in the place of $\partial /\partial t$. Then, on consideration of (2.12),
we may write for Eq.(2.4)'

$$(\frac{\partial}{\partial t} + \frac{\vec{p}}{m} \cdot \text{grad} - \text{grad } U \cdot \frac{\partial}{\partial \vec{p}}) \rho = 0 \tag{2.15}$$

This is the Liouville equation in the classical-mechanical
sense.

2. **The Liouville equation in the quantum-mechanical sense.**

From Eqs.(2.3) and (2.4), we may derive the Liouville
equation in the quantum-mechanical sense, as analogous to the
classical one. Since Eq.(2.3) contains a, we have to solve
the two equations simultaneously. Suppose that we have a set
of "complete" solutions which contain six arbitrary constants:

$$S(\vec{r}, t, \alpha, \delta) , \quad a(\vec{r}, t, \alpha, \delta)$$

where

$$\vec{r} \equiv x, y, z, \quad \alpha \equiv \alpha_1, \alpha_2, \alpha_3, \quad \delta \equiv \delta_1, \delta_2, \delta_3$$

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Then we define $\vec{p}$ and the β's by

$$\vec{p} = \text{grad } S \tag{2.16}$$

$$\beta_1 = -\partial S/\partial\alpha_1, \quad \beta_2 = -\partial S/\partial\alpha_2, \quad \beta_3 = -\partial S/\partial\alpha_3 \tag{2.17}$$

Here $\vec{p}$ is simply a vector variable and does not necessarily means momentum. According to (2.16), we have

$$p_x = p_x(\vec{r}, t, \alpha, \gamma)$$
$$p_y = p_y(\vec{r}, t, \alpha, \gamma) \tag{2.18}$$
$$p_z = p_z(\vec{r}, t, \alpha, \gamma)$$

and according to (2.17)

$$\beta_1 = \beta_1(\vec{r}, t, \alpha, \gamma)$$
$$\beta_2 = \beta_2(\vec{r}, t, \alpha, \gamma) \tag{2.19}$$
$$\beta_3 = \beta_3(\vec{r}, t, \alpha, \gamma)$$

We regard the β's as invariant, in the same way as in the classical case. By eliminating $\vec{r}$ from (2.18) and (2.19), we obtain

$$p_x = p_x(\alpha, \beta, \gamma, t)$$
$$p_y = p_y(\alpha, \beta, \gamma, t) \tag{2.20}$$
$$p_z = p_z(\alpha, \beta, \gamma, t)$$

and then, substituting the above in Eq.(2.18), we obtain

$$x = x(\alpha, \beta, \gamma, t)$$
$$y = y(\alpha, \beta, \gamma, t) \tag{2.21}$$
$$z = z(\alpha, \beta, \gamma, t)$$

$\vec{p}$ and $\vec{r}$ are independent, since they contain nine constants . (See the statement following Eq.(2.11).) Further, by solving (2.20) with respect to the α's and substituting the result in $a(\vec{r}, t, \alpha, \gamma)$, we obtain

$$a = a(\vec{r}, \vec{p}, t, \beta, \Gamma) \qquad (2.22)$$

If we substitute the above for a in Eq.(2.4) , operator $\partial/\partial t$
has to be read

$$\partial/\partial t + (d\vec{r}/dt)_r \cdot \partial/\partial \vec{p}$$

Hence, Eq.(2.4) yields

$$\frac{\partial a^2}{\partial t} + (\frac{d\vec{p}}{dt})_r \cdot \frac{\partial a^2}{\partial \vec{p}} + \frac{\vec{p}}{m} \cdot \frac{\partial a^2}{\partial \vec{r}} = 0 \qquad (2.23)$$

We may calculate $(d\vec{p}/dt)_r$ from Eq.(2.3) where t and $\vec{r}$ are
mutually independent. First, operate operator grad:

$$\partial (grad\ S)/\partial t + grad\ (grad\ S)^2/2m + grad\ U - \frac{\hbar^2}{2m} grad(\Delta a/a) = 0$$

Considering $\vec{p}$ = grad S, we obtain

$$(d\vec{p}/dt)_r + grad\ U - \frac{\hbar^2}{2m} grad(\Delta a/a) = 0 \qquad (2.24)$$

On eliminating $(d\vec{p}/dt)_r$ from (2.23) and (2.24), we have

$$\frac{\partial a^2}{\partial t} - (grad\ U - \frac{\hbar^2}{2m} grad(\Delta a/a)) \cdot \frac{\partial a^2}{\partial \vec{p}} + \frac{\vec{p}}{m} \cdot \frac{\partial a^2}{\partial \vec{r}} = 0$$
$$(2.25)$$

This may be regarded as the Liouville equation in the quantum-
mechanical sense.

It is noted that the Wigner equation, derived also from
the Schrodinger equation, is equivalent to the classical
Liouville equation to the approximation of nullifying $\hbar$,
not $\hbar^2$, if the potential U is expandable in a Taylor series of
distance and its first derivative is retained. See Ref.2.
The difference between the Wigner equation and Eq.(2.25) may
be attributed to the difference between the definitions of $\vec{p}$.
The present equation is more advantageous in the sense that
its connection to the classical one is explicit and natural.

We may perform the same reduction as in the above, with
respect to the Schrodinger equation for a many-particle system.

III. SOLUTIONS OF THE CLASSICAL
LIOUVILLE EQUATION

In the classical Liouville equation (2.15), variables
t, $\vec{r}$, $\vec{p}$ are independent. ($\vec{r}$ = x, y, z. $\vec{p}$ = p_x, p_y, p_z.)
Therefore, in general, a solution of the equation is a
function of those independent variables. As we change
arbitrarily the values of those variables, ρ changes accordingly.
If we impose a certain relation between those changes of
independent variables, however, ρ may not change. The relation
is given by the characteristic equations of Eq.(2.15):

$$dt = \frac{dx}{p_x/m} = \frac{dy}{p_y/m} = \frac{dz}{p_z/m}$$

$$= -\frac{dp_x}{\partial U/\partial x} = -\frac{dp_y}{\partial U/\partial y} = -\frac{dp_z}{\partial U/\partial z} \qquad (3.1)$$

In other words, if the changes occur according to (3.1),
ρ does not change. Equation (3.1) are the Newton equations
of dynamics. We note the following: Suppose that we have
a solution of Eq.(2.15), a function of $\vec{r}$, $\vec{p}$ and t. By equalizing
the solution to a constant, say A, we obtain an equation

$$\rho(\vec{r},\vec{p},t) = A$$

This equation should be satisfied by a set of solutions of (3.1).
But we cannot derive (3.1) from this equation.
In the following, we shall discuss three typical solutions
of Eq.(2.15):

1. <u>Solution for a single system.</u>

$$\rho_i = \rho_0 \, \delta(x - x(t)) \, \delta(y - y(t)) \, \delta(z - z(t)) \times$$
$$\times \delta(p_x - p_x(t)) \delta(p_y - p_y(t)) \, \delta(p_z - p_z(t))$$
$$(\rho_0 = \text{const})$$
$$(3.2)$$

This function, δ function, satisfies the Liouville equation (2.15), if $x(t)$, $y(t)$, $z(t)$, $p_x(t)$, $p_y(t)$, $p_z(t)$ are solutions of Eqs.(3.1), and x, y, z, p_x, p_y, p_z are independent variables. Function (3.2) represents a single system in the phase space.

2. Ensembles in general.

From (3.2), we may generate a solution which represents a group of similar systems (ensemble). In (3.2), those functions of time t

$$x(t), \; y(t), \; z(t), \; p_x(t), \; p_y(t), \; p_z(t)$$

contain their initial values denoted by

$$x_0, \; y_0, \; z_0, \; p_{x0}, \; p_{y0}, p_{z0}$$

If the initial density distribution of the group of the systems is given by

$$\varphi (x_0, \; y_0, \; z_0, \; p_{x0}, \; p_{y0}, \; p_{z0}) \tag{3.3}$$

then

$$\rho = \iiiint\!\!\!\int\!\!\int \varphi \rho_i \, dx_0 dy_0 dz_0 dp_{x0} dp_{y0} dp_{z0} \tag{3.4}$$

is the solution which we wish to obtain.

3. Micro-canonical ensemble.

If we take for ρ

$$\rho = a^2 = f(U + p^2/2m) \tag{3.5}$$

we see easily that this satisfies Eq.(2.15). In order to make this as the representation of a microcanonical ensemble, an additional condition is necessary, that is

$$U + p^2/2m = E = \text{const} \tag{3.6}$$

This is equivalent to taking for S in Eq.(2.3)'

$$S = - Et + s \qquad (3.7)$$

where E is constant and s is independent of t. By (3.7), equation (2.3)' yields

$$-E + p^2/2m + U = 0 \qquad (3.6)$$

In summary, the following are significant: a) The characteristic equations are independent of ρ . b) A characteristic line does not cross another line.

We may consider the same with respect to many-particle systems.

IV. SOLUTIONS OF THE SCHRODINGER EQUATIONS AND THE CORRESPONDING SOLUTIONS OF THE CLASSICAL LIOUVILLE EQUATION *

The Liouville eq.(2.15) is linear and of the first order. But equation (2.25) which may be called the quantal Liouville equation is neither linear nor of the first order.

We begin our investigation by assuming that $(h^2/2m)\mathrm{grad}\left(\frac{\Delta a}{a}\right)$ in the equation is a minor correction term. Then we may think that the classical equation (2.15) is the substitute of Eq.(2.25) to the first approximation. Then, on substitution of the first approximate solution of a in the correction term, we may consider Eq.(2.25) as linear and of the first order. After repeating successively similar processes of approximation, we may define a trajectory by

*Those speculations, made in this section and unnecessary in the standard quantum mechanics,are merely for the convenience for the discussion in section V.

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$$\frac{d\vec{p}}{dt} = - \text{grad } U + \frac{\hbar^2}{2m} \text{grad } \left(\frac{\Delta a}{a}\right)$$

$$\frac{d\vec{r}}{dt} = \frac{\vec{p}}{m}$$

(4.1)

These are characteristic equations of Eq.(2.25) to the present approximation. It is rather obvious that we cannot call a line, determined in the pahse space according to (4.1), as "trajectory" of a particle, because here the trajectory appears to be affected by a or by other systems and the situation is contradictory to the definition of ensemble that a system belonging to an ensemble should not be affected by another system belonging to the same ensemble. The only feasible interpretation is that the behavior of a system (a particle in this case) is represented by a bundle of those characteristic lines, instead of a single line. At a moment of time, a finite domain of the 6-dimensional phase space represents a state of a particle. According to the present interpretation, a^2 may be the representation of an ensemble of systems which do not interfere mutually, only when each finite domain of the relevant phase space representing a state of a system is separated from the others in function a^2 at each moment of time. One representative domain of the phase space should be occupied only by one system at a moment of time. (The situation is similar to the situation of many billiard balls which are on the same table and do not collide mutually.) If this condition is not satisfied, a trajectory may violently deviate from any of thephysically possible ones because of the interference which should not occur on a system in the ensemble, and the situation causes singularity of a^2.

Thus far, we have been assuming that we solve Eq.(2.25) by a method of successive approximation, simply for the

*A similar interpretation was proposed earlier by de Broglie. See Ref. 3 . The term containing a in (4.1) should belong to the concerned particle itself.

purpose of understanding the effect of the non-linear terms in
Eq.(2.25). The method of successive approximation is not prac-
tical, however: We do not know, in advance of solution, how should
the first approximation be set, such that the convergency of the
final result is assured. If we obtain an exact solution all at
once and the solution does not contain any singularity, we may
expect that the solution be physically significant.

  1. Energy Eigen-solutions.

  An energy eigen-function of the Schrodinger equation is
given by

$$\psi(x,y,z,t) = a \exp(iS/\hbar) \qquad (4.2)$$

where $\qquad S = -Et + s \qquad\qquad (4.3)$

and E is constant, s and a are independent of t. Then we have

$$i\hbar \partial\psi/\partial t = E\psi$$

On this understanding, we substitute (4.2) in Eqs.(2.3) and
(2.4), obtaining

$$-E + U + (\text{grad } s)^2/2m - \hbar^2 \Delta a/(2ma) = 0 \qquad (4.4)$$
$$\partial a^2/\partial t = 0, \quad \text{div}(a^2 \text{grad } s/m) = 0 \qquad (4.5)$$

According to the definition of $\vec{p}$ made in section II, we may
rewrite (4.4) and (4.5), and obtain*

$$-E + U + p^2/2m - \hbar^2 \Delta a/(2ma) = 0 \qquad (4.4)'$$
$$\left.\begin{array}{c} \partial a^2/\partial t - [\text{grad } U - (\hbar^2/2m)\,\text{grad}(\Delta a/a)]\cdot\partial a^2/\partial\vec{p} = 0 \\ \vec{p}\cdot\text{grad } a^2 = 0 \end{array}\right\} \qquad (4.5)'$$

Due to the introduction of p, a may be a function of t.

  If we nullify $\hbar^2$ in the above, Eq.(4.4)' implies the energy
conservation in the classical sense, and this condition determines
a surface in the phase space. On the surface, a^2 may change in
such a way that Eqs.(4.5)' are satisfied. This is the represent-
ation of a microcanonical ensemble. As far as those conditons
are satisfied, we may choose the distribution of a^2 arbitrarily.

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*If a is independent of $\vec{r}$, we have

$$i\hbar \partial\psi/\partial\vec{r} = (\text{grad } s)\psi = \vec{p}\,\psi$$

In this case, $\hbar^2 \Delta a/(2ma)$ in (4.4)' disappears.

The situation is shown by Eq.(3.5), where we may choose function
f and E as we wish. a^2 (or f) represents a superposition of
various trajectories possible under condition (3.6).

If the term containing h in Eq.(4.4)' is significant, the
distribution of a also affects the energy law of the system
under consideration (a particle in this case). According to the
interpretation made in the beginning of this section, a feasible
solution is expected to exist only under a restrictive condition.
Indeed, according to Schrodinger, the possible values of E, in
the case of an electron in an atom for example, are strictly
specified, and only for each of such values of E, a^2 and S are
possible to be determined uniquely, with no singularity. An
eigen function thus determined in the configuration space gives
us only a vague information of the behavior of the system under
consideration. The vagueness stems from two causes: 1) The
state of a particle at a moment of time is represented by a^2
and S in a finite domain of the phase space, and consequently
a trajectory of the particle, not only in the configuration
space but also in the phase space, is not a line but a bundle
of lines. 2) Many possible trajectories, each representing
a possible and entire history (cycle) of the system, are
superposed in one configuration space, as well as in the relevant
phase space, and represent a microcanonical ensemble*. (The
first cause is found only in a quantum-mechanical system. But
the second cause exists also with respect to a classical system.)
Thus a^2 appears to represent a cloud spread in the entire
configuration space. The present interpretation is obviously
different from Born's interpretation**. Born attributed the
peculiar characteristic of the cloud, which is partly (or mainly?)
the characteristic of an ensemble even in the classical sense,

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*In the Schrodinger solution, the magnitude and direction
of angular momentum are also specified.. But the direction of
apogee is not spacified.

**The reader may complain the author, because our inter-
pretation produces nothing new so far as the standard problems of
quantum mechanics are concerned. But in section V, we shall see
the significance.

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to the assumed peculiarity of quantum-mechanical particles.
See Ref. 5. (In his classical kinetic theory, Born is not sensitive
of ensemble. Ref.1.)

2. <u>Wave packet and plane wave.</u>

It is often said that a wave packet which satisfies
the Schrodinger equation represents a free particle.
If $U = 0$ in the Schrodinger equation (2.1), we have for
a solution

$$\exp (i\ p_x x/\hbar - i Et/\hbar) \tag{4.6}$$

$$E = p_x^2/2m \tag{4.7}$$

Consequently, the Fourier transform of G, a function of
p_x/mc

$$\psi(xt) = \int_{-\infty}^{+\infty} G(p_x/mc)\exp(i\frac{p_x x}{\hbar} - i\ \frac{Et}{\hbar})\ d(p_x/mc)$$

$$\tag{4.8}$$

is also a solution. If we choose G properly, ψ represents
a localized wave (one-dimensional wave packet), although
unstable*. See Ref.6. At the limit $\hbar \to 0$, the wave packet
appears to be a plane, placed perpendicularly to the x-
axis and moving in the x-direction. We may construct a
three-dimensional wave packet which may represent a
particle.

If we distribute many similar wave packets in the
three-dimensional configuration s pace, and the distribution
is made with a certain regularity as depending on function G,
we obtain a plane wave to an approximation:

$$\psi = a\ \exp (i\ p_{x0}x/\hbar - i\ E_0 t/\hbar) \tag{4.9}$$

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* Schould this instability be attributed to the nature
of a particle or to the imperfection of the Schrodinger
equation? Some arbitrariness permissible in the choice of G
suggests the latter.

where p_{x0}/m is the group velocity of a packet, and $E_0 = p_{x0}^2 /2m$. Since amplitude a in (4.9) is substantially constant, the corresponding classical ensemble consists of similar one-particle systems distributed uniformly in the 3-dimensional configuration space. At this classical limit, we cannot detect the regularity or order given primarily to the distribution of the wave packets, as necessary for forming the plane wave (4.)). In an ensemble, each system (a particle in this case) should not interact with any other system (a particle), no matter how closely may they be located in the space. This demand of the definition of ensemble and the conventional mathematical scheme of representation are compatible, so far as classical material points are concerned. But it is not so with respect to quantal particles, as is manifest in Eq.(4.1). The regularity imposed on the distribution of wave packets is a mathematical convenience, but is an unnecessary restriction from the view-point of physics. For example, if we suppose that a beam of electrons is represented by an ensemble of single-particle systems, the only necessary condition is that each electron in the beam is independent of the others. We cannot expect that the distribution of those electrons in the beam should be regulated in the same way as the distribution of those wave packets is for making a plane wave. In other words, a plane wave is simply a representation of a single particle for a certain purpose specified in quantum-mechanics.

As Dr. Ruark once pointed out to the author, those speculations made in this section are all unnecessary(meaningless) for solving the conventional problems of quantum-mechanics. Nothing, new and significant, may be developed from them. They may be rather disgustful in the sense that that miracurous beauty and perfection of the system of quantum mechanics be unnecessarily destroyed by them. Nevertheless, the author thinks that those speculations are necessary for solving kintic-theoretical problems such as demonstrated in the next section.

V. FROM THE KINETIC-THEORETICAL
VIEW POINT

Thus far, we have seen that there are good mathematical
correspondences between quantum-mechanical solutions of the
Schrodinger equation and ensemble solutions of the classical
Liouville equation. Thus far, however, we have not said
that those solutions of the Schrodinger equation represent
ensembles. For it is merely nominal and insignificant to do
so from the physical view point, so far as those conventional
solutions are concerned. In the following, however, we shall
show that <u>the same physical significance as seen of the differ-</u>
<u>ence between ensemble and single system in classical mechanics</u>
<u>is also found of the difference between mathematically nomi-</u>
<u>nated   ensemble and mathematically nominated   single</u>
<u>system in quantum mechanics treating a kinetic phenomenon.</u>

We suppose that we have two similar electron beams in a
large vacuum chamber. Each of them is well collimated. One
beam is set along the x-axis and the other along the y-axis of
our imaginary coordinate system. We may call them respectively
the X beam and the Y beam. They intersect mutually in the
domain surrounding the origin of the coordinate axes. We
wish to investigate the mode of the interaction by means of the
Schrodinger equation. Quantum mechanics suggest the following
two methods:

<u>Method I.</u>

We represent each of the two beams with a plane wave, to
the zeroth approximation: The X beam with ψ_x^o and the Y beam
by ψ_y^o. It is obvious that $\psi_x^o \psi_y^o$ satisfies the relevant
Schrodinger equation where the interaction term is neglected.
(There are only two independent coordinate variables x, y in
the equation.) To the next approximation, we substitute
$\psi_x^o \psi_y^o$ in the interaction term and $\psi_x^o \psi_y^o + \varphi$ in the other terms

of the Schrodinger equation. Thus we have a partial differntial
equation where ψ is unknown. φ gives the effect of the interaction
between the two beams. Although we do not solve the equation for
ψ in this report, it is not difficult to guess the essential
characteristic of the result. The beams are both retarded as
they approach toward the intersection and are accelerrated after
leaving the intersection. The effect of crossing is expected
only in a space near the intersection. (Also we have to consider
the interaction between one part of a beam and another part of
the same beam. This effect has no direct relation to the purpose
of the present discussion. Note,the beams are well collimated.)
The interaction is very smooth; there is no abrupt interaction.

Method II.

We assume, to the zeroth approximation, that each electron
is represented by a wave packet. (Since the velocity of each
beam is large and our observation is limited to the vicinity of
the intersection, each packet may be assumed to be stable.)
Each beam consists of many similar wave packets, in the same
way as a gas consists of classical molecules. The wave function
of the whole system is the product of all the wave-packet
representations:

$$\psi^{\circ} = \prod \psi_n^{\circ} \qquad n=1,2,3,\ldots\ldots$$

ψ° satisfies the Schrodinger equation where the interaction
terms are neglected. It should be noted that, unlike the case
of Method I, the independent variables are t, and x_1, x_2, x_3,..
for the X beam and y_1, y_2, y_3,.. for the Y beam. Each wave packet
contains t and one spatial coordinate. Therefore, the Schrodinger
equation contains many interaction terms for all the pairs of
those coordinates. To the next approximation, we do the same
as we did in Method I. ψ° is substituted in the interaction

terms, and $\psi^o + \psi$ in the other terms of the Schrodinger
equation. Here again, we do not solve the equation. But
we can predict the result according to our experience of
classical gas theory. In this case, the energy, momentum and
charge of each electron are not spread over the entire beam,
but instead are concentrated within a tiny wave packet. Hence
there is a possibility that an electron in the X beam and an
electron in the Y beam interact violently and abruptly, like
two particles colliding according to the classical dynamics.
As a result, an electron after interaction may not stay in
the beam where it belongs; instead it may run out to a complete-
ly different direction. The detail is fairly well known by
the classical kinetic theory, and is omitted here.

After studying comparatively the two methods, we realize
that, the physical characteristic of problem I is quite
similar to the characteristic of the problem of treating a
classical-mechanical system in terms of its ensemble represent-
ation. On the other hand, the situation in problem II is
similar to the situation of a classical mechanical system
when treated as a single system. (In classical kinetic theory,
ensemble representation is not useful. See Ref. 1.)

We may now believe that the correspondence found in section
IV does not remain merely as mathematical, but the correspondence
manifests itself in physical phenomena. Our conclusion is
that those speculations made in section IV have physical signifi-
cance, when we investigate kinetic-theoretical phenomena which
have been being ignored by the conventional quantum mechanics.

The reader might ask, what is the feasible approach of
kinetic theory? The possible and most reasonable way, at this
time, of kinetic theory seems to rely on quasi-classical models
of particles. There is a reason for being optimistic about
this approach: A system which we are interested in from the
kinetic-theoretical view-point tends to contain a comparative-

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ly large amount of energy, and quasi-classical models may well simulate real particles consituting the system.

VI. CONCLUDING REMARK

In this report, our interpretation of quantum-mechanical phenomena has gone somehow beyond the standard one, and possibly might have provoked some uneasiness in the reader. However, we should note that the present discussion has done nothing to antagonize the authorized or standard interpretation of quantum mechanics, so far as the conventional problems are concerned. As is simply stressed in section V, if we wish to investigate a group of phenomena, which may be called kinetic-theoretical, we have to make up an interpretation which is compatible with the standard one and yet possible to give feasible solutions for those strange problems. This is what we have discussed in this report. If the reader could take the matter in this sense, the author would be most grateful.

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APPENDIX
A COMPLETE SET OF ORTHOGONAL EIGEN FUNCTIONS
IN THE CONFIGURATION SPACE AND IN THE PHASE SPACE

In the following, $\vec{p}$ does not mean momentum in the classical sense, but instead is simply a variable defined by (2.16). Hence, the discussion is merely mathematical, so far as this section is concerned. However, it has physical meanings when coope rating with section V.

According to Eqs.(4.2) and (4.3), we write those eigen functions as follows:

$$\psi_k = a_k \exp(-iE_k t/\hbar)\exp(is_k/\hbar) \tag{A.1}$$

$$k = 1,2,3,\ldots$$

Here, E_1 , E_2 , ... are respectively constants, and a_1 , s_1 , a_2 , s_2 ,... are functions of $\vec{r}$ = x,y,z while being independent of t. However, if we introduce $\vec{p}_1$, $\vec{p}_2$,... as defined by (2.16) a_k, s_k appear to be dependent of time t, as is shown by (4.5)'. This is due to a transformation among invariants as is stated with respect to (2.22):

$$a_k(\vec{r},\alpha_k, \gamma_k) = a_k(\vec{r},\vec{p},t, \beta_k, \gamma_k)$$
$$s_k(\vec{r},\alpha_k, \gamma_k) = s_k(\vec{r},\vec{p},t, \beta_k, \gamma_k) \tag{A.2}$$
$$k = 1,2,\ldots$$

In the rp-space, function $a_k(r,\alpha_k, \gamma_k)$ is an envelope of function $a_k(r,p,t, \beta_k, \gamma_k)$ as is illustrated schematically in Fig.1.

Since the E's are constants, the orthogonal relations among the ψ's are given by

$$\int a_k a_{k'} \exp\left[i(s_k - s_{k'})/\hbar\right] dr = 0 \tag{A.3}$$
$$k \neq k'$$

In the configuration space (r-space), each function $a_k(r,\alpha_k,\gamma_k)$ covers the entire space. But in the pr-space, they are separable.

As we know well, the domains are completely separable in the classical case. But, because of a involved in Eq.(4.4)', they may be partly overlapped in this case. Nevertheless, at each moment of time, they are distingui;shable if p is defined by

$$\vec{p}\,(r,t,\beta_k,\delta_k) \tag{A.4}$$

according to (2.20) and (2.21), where (β_k,δ_k) is different from one eigenfunction to another. The situation is schematically illustrated in Fig.2.
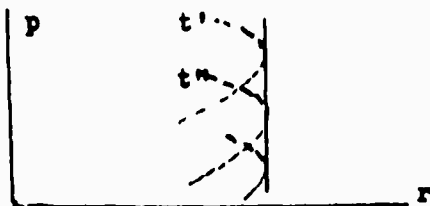

Fig.1. The solid line represents $a_k(r,\alpha_k,\delta_k,)$=const. Each dotted line represents $a_k(r,p,t,\beta_k,\delta_k)$=const. at each different time, t', t",...
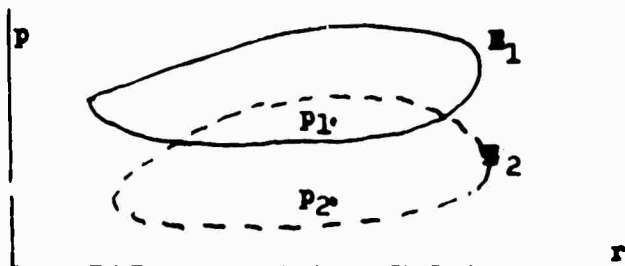

Fig.2. The domain of eigenfunction of E_1 is represented by the domain enclosed by solid line, and the domain of eigenfunction of E_2 by the domain by dotted line. Since a is involved in Eq.(4.4)', they may be overlapped, in general. But, if r and t are given, the values of p, (A.4), are different in two cases of E.

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13. ABSTRACT

The theme of this report is a problem of correlation, as is illustrated in section I by considering the two-electron problem according to the Schrodinger equation. In section II, the Schrodinger equations is reduced to a partial differential equation which is equivalent to the classical Liouville equation, to the approximation of nullifying h^2 in the former. An energy eigen-function of the Schrodinger equations corresponds to the representation of a microcanonical ensemble of classical-mechanical systems in the phase space. For example, the energy eigne function of the electron in a one-electron atom corresponds to a microcanonical ensemble of single-particle systems in the classical mechanical sense. The uncertainty existing in the quantum-mechanical representation of a particle is two-fold: A part of the uncertainty stems from our intention to describe the behavior of the particle,which is likely to have an extension in the six-dimensional phase-space, in terms of the concept of classical material point; it also stems from the situation that we are treating an ensemble when we assumed that we are treating a single particle. If this were not the case, we would have no way to explain strange kinetic-theoretical phenomena, which really exist and fail to arise from the application of conventional theories. In view of the above, the kinetic theory of quantum-mechanical systems is difficult to rely on standard solutions of the Schrodinger equation. Rather, at the present time, it seems most reasonable to utilize quasi-classical models of particles. The present discussion provides some legitimacy and significance to those models. Finally, the present

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Abstract (Continued)

interpretation of quantum mechanical phenomena provokes no dis-
turbance in the conventional structure of the quantum-mechanical
interpretation of the Schrodinger equation, so far as the
conventional application of the solutions of the equation are
concerned.